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GEN IV MATERIALS HANDBOOK IMPLEMENTATION PLAN

Philip Rittenhouse and Weiju Ren

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ACRONYMS

AFCI	Advanced Fuel Cycle Initiative
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
DOE	The Department of Energy
DOE-NE	DOE's Office of Nuclear Energy
GFR	gas-cooled fast reactor
GIF	Generation IV International Forum
GUI	graphic user interface
HTML	hypertext markup language
I-NERI	International Nuclear Energy Research Initiative
ID	identification number
INL	Idaho National Laboratory
IT	information technology
LFR	lead-cooled fast reactor
MFR	master functional requirement
MSR	molton salt reactor
NE	Nuclear Energy
NGNP	Next Generation Nuclear Plant
NHI	Nuclear Hydrogen Initiative
NRC	Nuclear Regulatory Commission
NTD	national technical director
ORNL	Oak Ridge National Laboratory
PSF	product security functionality
QA	quality assurance
R&D	research and development
SCWR	supercritical water reactor
SFR	sodium-cooled fast reactor
SI	sulfur iodine
SIMs	system integration managers
UI	user interface
UNS	United Numbering System
VHTR	very high temperature reactor
VPN	Virtual Private Net

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Executive Summary

A *Gen IV Materials Handbook* is being developed to provide an authoritative single source of highly qualified structural materials information and materials properties data for use in design and analyses of all Generation IV Reactor Systems. The *Handbook* will be responsive to the needs expressed by all of the principal government, national laboratory, and private company stakeholders of Gen IV Reactor Systems. The *Gen IV Materials Handbook Implementation Plan* provided here addresses the purpose, rationale, attributes, and benefits of the *Handbook* and will detail its content, format, quality assurance, applicability, and access.

Structural materials, both metallic and ceramic, for all Gen IV reactor types currently supported by the Department of Energy (DOE) will be included in the *Gen IV Materials Handbook*. However, initial emphasis will be on materials for the Very High Temperature Reactor (VHTR). Descriptive information (e.g., chemical composition and applicable technical specifications and codes) will be provided for each material along with an extensive presentation of mechanical and physical property data including consideration of temperature, irradiation, environment, etc. effects on properties. Access to the *Gen IV Materials Handbook* will be internet-based with appropriate levels of control. Information and data in the *Handbook* will be configured to allow search by material classes, specific materials, specific information or property class, specific property, data parameters, and individual data points identified with materials parameters, test conditions, and data source. Details on all of these as well as proposed applicability and consideration of data quality classes are provided in the *Implementation Plan*.

Website development for the *Handbook* is divided into six phases including 1) detailed product analysis and specification, 2) simulation and design, 3) implementation and testing, 4) product release, 5) project/product evaluation, and 6) product maintenance and enhancement. Contracting of development of the *Handbook* website is discussed in terms of host server options, cost, technology, developer background and cooperative nature, and company stability. One of the first and most important activities in website development will be the generation of a detailed *Handbook* product requirements document including case diagrams and functional requirements tables.

The *Implementation Plan* provides a detailed overview of the organizational structure of the *Handbook* and details of *Handbook* preparation, publication, and distribution. Finally, the Implementation Plan defines Quality Assurance requirements for the *Handbook.*

1. Objectives of the Gen IV Materials Handbook Implementation Plan

The *Gen IV Materials Handbook Implementation Plan* is being prepared to outline and discuss the goals and objectives of the *Gen IV Materials Handbook* (hereinafter in text the *Handbook*) and how these will be achieved. The *Implementation Plan* will address and explain the purpose, rationale, attributes, and benefits of a single, authoritative Gen IV materials database contained in the *Handbook*. It will also detail the structure, content, format, and applicability of the *Handbook* and how access to the *Handbook* will be achieved and controlled. The Organizational Structure necessary to guide and operate the *Handbook* will be described as well as the procedures for its preparation, publication, and distribution. Finally, the aspect of Quality Assurance necessary for the *Handbook* will be discussed.

2. Purpose of the Gen IV Materials Handbook

The structural materials property data and associated materials information that are used in all phases of design, analysis, etc., of Gen IV Reactor Systems must be internally consistent, validated, and highly qualified. A materials database handbook serving as an authoritative single source of such data is a proven logical, efficient, and effective method for meeting the requirements above and for further assuring consistency of property values used by all stakeholders. Examples of such handbooks are the *Nuclear Systems Materials Handbook* developed in the past for DOE's Breeder Reactor Program and more recently the *AFCI Materials Handbook*. It is intended that the *Handbook* developed for use by Gen IV will provide all of the data attributes noted above and further ensure that materials data are available at the earliest possible time as input to preliminary designs and design comparisons. The *Handbook* will also provide an assessment of the quality of the record of materials properties included.

The results and findings of a Gen IV Materials Handbook Workshop held on July 28-29, 2004 in La Jolla, California provided additional support and rationale for the existence of the *Handbook*. The subject workshop was attended by the principal stakeholders of the *Handbook* including senior materials managers/experts from the reactor vendor community (General Atomic, General Electric, Areva, and Pebble Bed Modular Reactor), representatives from relevant American Society of Mechanical Engineers (ASME)/American Society of Testing and Materials (ASTM) standards and code committees, the Section Head for the Nuclear Regulatory Commission (NRC) Office of Nuclear Regulatory Research, the Department of Energy (DOE) Gen IV Program manager, Gen IV System Integration Managers (SIMs), and materials experts and managers from Oak Ridge National Laboratory (ORNL). The participants were unanimous in strongly supporting a DOE-led materials handbook/database activity with particular initial focus on Next Generation Nuclear Plant (NGNP) materials. Further, such an activity would be an excellent opportunity for international collaboration and thereby provide for the inclusion of valuable materials data from other Gen IV international partners. However, it was agreed that implementation of such international cooperation will not be initiated until the *Handbook* is more fully established. It was also emphasized the *Handbook* is not intended to serve as a substitute for ASME/ASTM

codes and standards but is to provide an out-in-front source of materials data that will contain more extensive data and information than is provided in these codes and standards.

3. Scope of the Gen IV Materials Handbook

The *Handbook* is intended to include structural materials necessary for the design and construction of Gen IV candidate reactor systems. These are

- The Supercritical Water Reactor (SCWR)
- The Very High Temperature Reactor (VHTR/NGNP)
- The Gas-Cooled Fast Reactor (GFR)
- The Lead-Cooled Fast Reactor (LFR)
- The Sodium-Cooled Fast Reactor (SFR)
- The Molten Salt Reactor (MSR)

Further, structural materials necessary for related programs on the Advanced Fuel Cycle Initiative (AFCI) and the Nuclear Hydrogen Initiative (NHI) will also be included in the *Handbook.* The initial emphasis will be to include materials potentially important to the NGNP.

3.1 Materials and Materials Classes to Be Included

Candidate and alternate structural materials for various reactor components and applications are listed in Reference 1 for the NGNP, the SCWR, the LFR, and the GFR. Most of the metallic materials identified fall under the classes or categories of ferritic alloy steels, ferritic-martensitic steels, austenitic stainless steels, and Ni-base alloys. There is considerable overlap in materials in the various systems. For example, Alloy 800H is a serious candidate for application in the NGNP, the LFR, and the GFR and is not excluded for consideration in the SCWR. There are a few instances in which candidate metallic materials fall outside the general categories listed above. For example, both Ti alloys and Zircaloy 4 are candidates for special applications in the SCWR and refractory alloys may be used in the LFR. Further, there are many applications of non-metallic structural materials (graphites, carbon/carbon composites, ceramics, and ceramic composites) for the NGNP and the GFR. It is expected that materials of interest to both NHI and AFCI will also be included in the *Handbook*. Materials to be applied in the NHI are listed in Reference 2; they mirror in most respects the metallic and non-metallic materials described in Reference 1 for the Gen IV systems. Reference 3 describes materials for the AFCI**.** They form a subset of the materials of interest covered in References 1 and 2.

Based on this identification of materials of importance, it is suggested that materials entries into the *Handbook* be divided into metals and non-metals (Volumes I and II, respectively). Further, they should be provided independent of the system (i.e., not specific to any of the Gen IV reactor systems). Non-metals will be further divided as “graphites and carbon composites” and “ceramics and ceramic composites”. Categories

best suited to incorporate the materials identified in Reference 1 through 3 are the "ferritic alloy steels", "ferritic-martensitic steels", "austenitic stainless steels", "Ni- and Co-base alloys", "refractory and other alloys", and "welding filler metals".

Serious consideration was given to arranging the *Handbook* inputs according to the Unified Numbering System (UNS) for metals and alloys. The UNS has been in use since about 1975 and arranges alloys in 17 general categories ranging from A00001-A99999 (aluminum and aluminum alloys) through W00001-W99999 (welding filler metals). However, the metallic materials described in References 1 through 3 represent only a very few of these categories. Further, most of the many developmental alloys given in these same references do not yet have specific UNS numbers. Also, most non-materials specialists are relatively unfamiliar with the UNS designations (e.g., they typically would not know what UNS number or numbers to select to address an alloy or alloy class). For this reason, the UNS will not be used as the major indexing system in the *Handbook*. The UNS numbers for specific alloys will, of course, be provided in the *Handbook* along with other information on standards where available.

3.2 Materials Properties and Other Information to Be Included

For each material in the *Handbook* the following information will be provided.

- Description of the characteristics of the material (e.g., usual applications, crystal structure and phases present, and response to heat treatment)
- Chemical composition
- Relationship of processing and structure (e.g., effect of architecture in composite materials) on properties.
- Product forms and sizes available
- Applicable ASTM, ASME, and other technical specifications and Code Cases
- Physical and thermal properties (e.g., melting point/range, density, thermal conductivity, electrical resistivity, thermal expansion, specific heat, and emissivity)
- Elastic properties including Young's Modulus, Poisson's Ratio, and shear modulus
- Mechanical properties (tensile and compression properties, high- and low-cycle fatigue and creep-fatigue behavior, fracture toughness, creep and cyclic crack growth rates, and creep properties).

The temperature dependence of all available physical, thermal, elastic, and mechanical properties above will generally be provided. Information will also be given relative to corrosion, environmental effects, and thermal aging and the influence of all of these on materials properties. Another important consideration for many applications is the effect of irradiation on materials properties and this will also be made available in the *Handbook*. Finally, means of assessing the range of property values and the uncertainty of a specific property under specific conditions will be provided in the *Handbook*.

The materials properties data in the *Handbook* will be displayed in table form whenever possible. However, the *Handbook* will be constructed to permit data and information to be presented through the use of text, tables, figures, equations, and photographs as appropriate.

3.3 Access and Input to the *Gen IV Materials Handbook*

Some of the attributes of the *Handbook* relative to its accessibility and control are described in the bullets below.

- The *Handbook* will be web-based and available through the Internet with one or more distinctive addresses.
- Ordinary access to the *Handbook* beyond the Home Page will be controlled by passwords issued to individuals by *Handbook* management. This will be designated as Access Level #1.
- Any proprietary data/information or other data/information to be held confidential as a result of program agreements will be further protected by second-level passwords also issued by *Handbook* management. This will be designated as Access Level #2. Based on the data/information protection agreements, Access Level #2 can be further divided into various sections such as Access Level #2A, Access Level #2B, … etc.
- Access for input to the *Handbook* (additions, corrections, deletions, modifications, format changes, etc.) will be permitted only by a selected few approved by *Handbook* management. This will be designated as Access Level #3. All inputs will be subject to Gen IV Program Change Control. Records of changes will be maintained.
- The three passwords for different Access Levels can also be issued as a single password with 3 different Access Privilege Levels. A password of Access Privilege Level 1 can only log into Access Level # 1, while that of Access Privilege Level 3 can log into all three Access Levels.
- Passwords for all three levels of access will be carefully controlled and records of their issue will be maintained. When necessary, the use of security encryption schemes, such as Virtual Private Net (VPN), control will be considered.
- Access to the *Handbook* at all levels of access will allow the ability to download the data/information in both the original and print-friendly formats.
- The *Handbook* will satisfy all aspects of Gen IV Materials Quality Assurance.

3.4 Search Characteristics and Capabilities in the *Gen IV Materials Handbook*

This section outlines and discusses the protocol that is planned to permit navigation through the *Handbook* to arrive at a display of the data or information desired. Figure 1 shows the scheme or route that is anticipated to be followed in gaining this end point for a particular property over a range of parameters for a particular material. For example, this might be the "average" uniform tensile elongation at 700^{o}C for Alloy 800H irradiated to 1 dpa. Figure 2 addresses the protocol for accessing and assessing the individual data

points that make up this "average" value. This will include a means of statistical treatment of the data from which the "average" was derived, identification of the material parameters (product form, heat treatment, heat number, etc.) associated with each data point, identification of the test conditions (strain rate, etc.) under which each data point was acquired, and identification of the data source or reference for each data point. Figure 2 also shows a route for call up of the text of each reference. However, the very large scope of this latter endeavor will result in its implementation in the later phases of *Handbook* development.

The following example will be used to permit a better understanding of the protocols noted in the paragraph above and listed in Figures 1 and 2. The assumption here is that the primary interest is the range of values of the ultimate tensile strength of Ni-base alloys (Alloy 617 in particular) at 850^{o}C. One would proceed through Figure 1 as follows.

- Access the *Handbook* through its web address and enter using the assigned password or passwords.
- Search for "metals" (Volume I) in the *Handbook*.
- Search by "materials class" to determine the Ni-base alloys covered in the *Handbook* or bypass this step if a specific alloy is desired.
- Search by "material", in this case Alloy 617.
- After call up of Alloy 617, one can search by "general information" with access to such things as alloy chemistry and material specifications or by material property. In this example, the mechanical property "property class" will be called up.
- Search for ultimate tensile strength under "specific property".
- One could now search for the ultimate tensile strength values of Alloy 617 under all temperature, environmental, and irradiation conditions. However, for the particular interest in this example, it is only necessary to search for the ultimate tensile strength at 850^{o}C.

At this point the *Handbook* would display the mean value of the ultimate tensile strength of Alloy 617 at 850^{o}C +/- 25^{o}C. To obtain a more thorough understanding of the ultimate tensile strength behavior of the material, one must proceed as will be described in Figure 2.

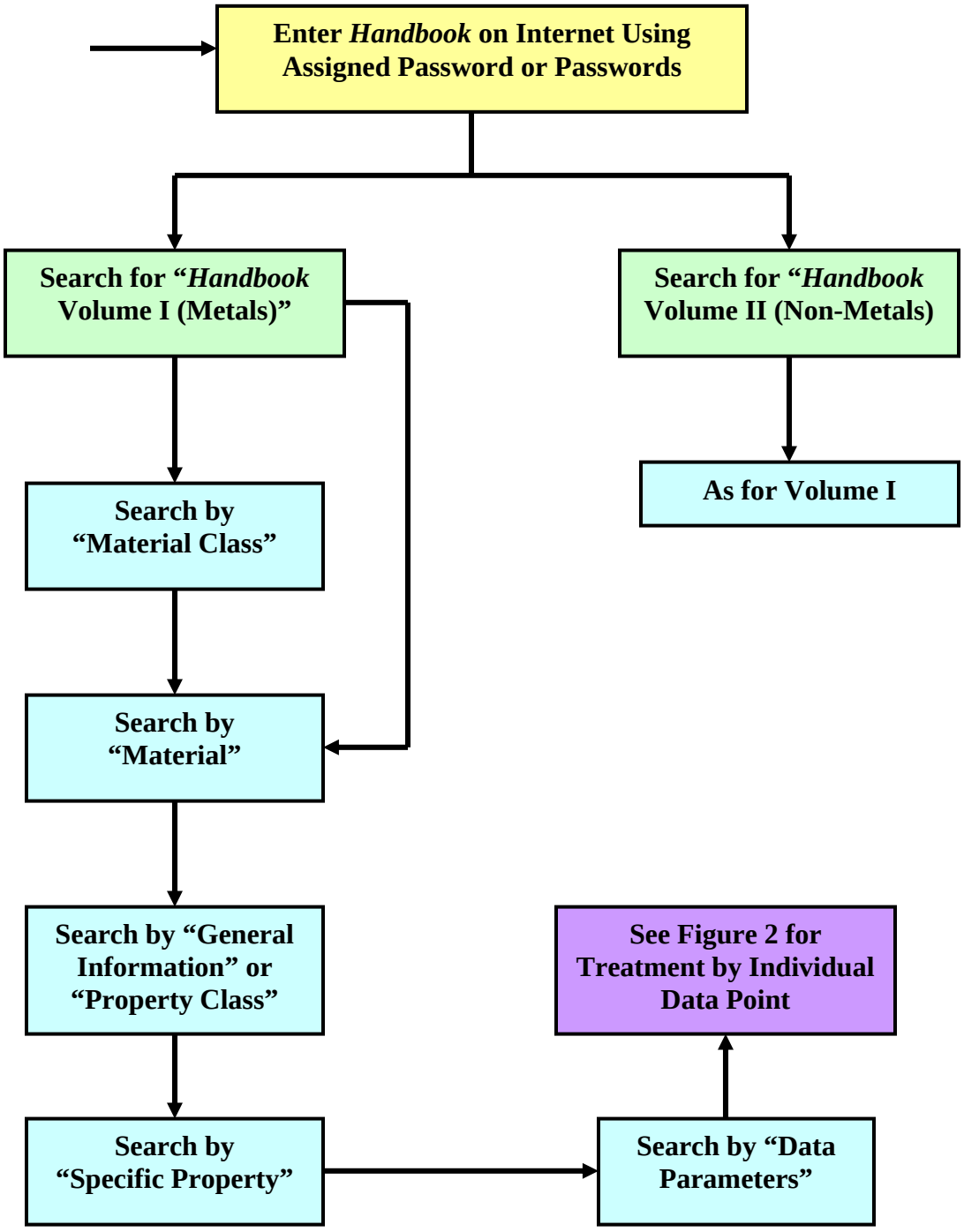

Figure 1. Outline of Protocol for Accessing Information in the Gen IV Materials Handbook

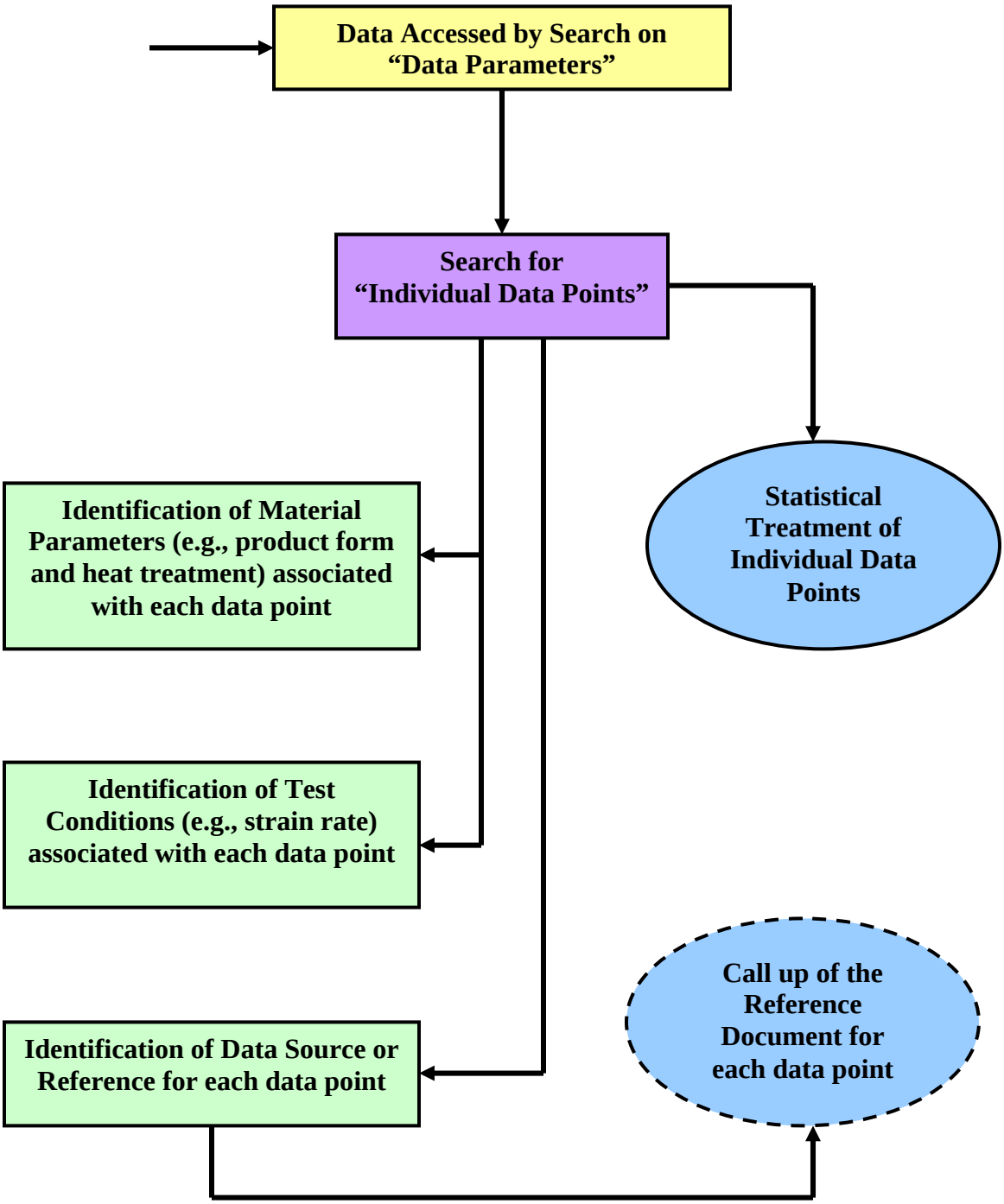

Figure 2. Outline of Protocol for Accessing and Assessing Individual Data Points in the Gen IV Materials Handbook

The variability or range of values of a materials property determined under nominally identical conditions (temperature, etc.) is extremely important to such considerations as setting allowable stresses, selecting "safety factors", and performing analyses relative to failure probabilities. For these reasons, it is important to include in the *Handbook* the capability to statistically treat the property data. Further, in order to fully understand the variability of a material property, it is necessary to identify each data point relative to a number of factors. These include "materials parameters" (e.g., product form, heat treatment and environmental exposure conditions, and alloy chemistry) and test conditions (specimen geometry, strain rate, test temperature, etc.). Finally, the source of each data point is important for traceability and quality purposes. This treatment of a material property by individual data point is displayed in Figure 2. First, the "data parameter" search for a particular mechanical property of a given material under specified conditions (described in reference to Figure 1) results in a mean value. In the current example, this is the mean value of the ultimate tensile strength of Alloy 617 at 850^{o}C +/-25^{o}C. The steps in addressing material property variability, etc. are as follows:

- Call for the "individual data points" forming the basis of the mean value from the "data parameters" search. Based on the example, this will provide all of the data points existing in the *Handbook* for the ultimate tensile strength of Alloy 617 tested at 850^{o}C +/-25^{o}C.
- If desired, each data point can be identified with specific "material parameters".
- If desired, each data point can be identified with specific "test conditions".
- A "statistical treatment" of the "individual data points" can then be performed using tools in the *Handbook*. In this case, this could be for all of the 850^{o}C+/-25^{o}C ultimate tensile strength data for Alloy 617 forming the overall mean or for groups of 850^{o}C+/-25^{o}C data points selected on the basis of common "test conditions", and/or "material parameters", and under more restrictive temperature conditions (e.g., 850^{o}C+/-10^{o}C).
- If desired, each data point can be identified with its "data source/reference".

Figure 2 shows a search on "data source/reference" to call up the associated documents for inspection. Getting these documents into electronic form for incorporation in the *Handbook* would be a significant effort and is not an early priority.

4. Web-Accessible *Gen IV Materials Handbook*

4.1 Basic Structure of the *Handbook*

There are many types of web-accessible databases. These range from static hypertext markup language (HTML) pages with no database support to dynamic ones with very complicated interactions with the end users. For the *Handbook*, a Three-Tier/N-tier model structure is anticipated to provide centralized common services in a distributed environment. A schematic of the Three-Tier/N-tier model is shown in Figure 3. The Data Tier is dedicated to data storage where the data are stored in various category tables such as microstructure image data, physical properties data, mechanical properties data etc., ready for processing. These category tables can be defined and arranged as needed.

The Application Tier consists of dedicated computing machines and application programs called servers. The Application Tier accesses the Data Tier to fetch, store, delete or change the data through four basic queries, namely SELECT, INSERT, UPDATE and DELETE. Through these four basic queries and the application programs, the Application Tier can process the data as instructed by the user. Various kinds of data processing tasks such as data analysis, curve fitting, data background review, etc. can be carried out through customized application programs in the Application Tier. Access control and other business rules and logics are also implemented in this tier. The Presentation Tier is composed of servers and the Graphic User Interface (GUI) programs. Through the GUIs, the Presentation Tier can display processed data in required formats and forms and create links that the end user sees on the web page. They also serve as interaction ports with the user. The model in Figure 3 is some time referred to as N-tier model because the Application Tier may consist of multiple layers of servers.

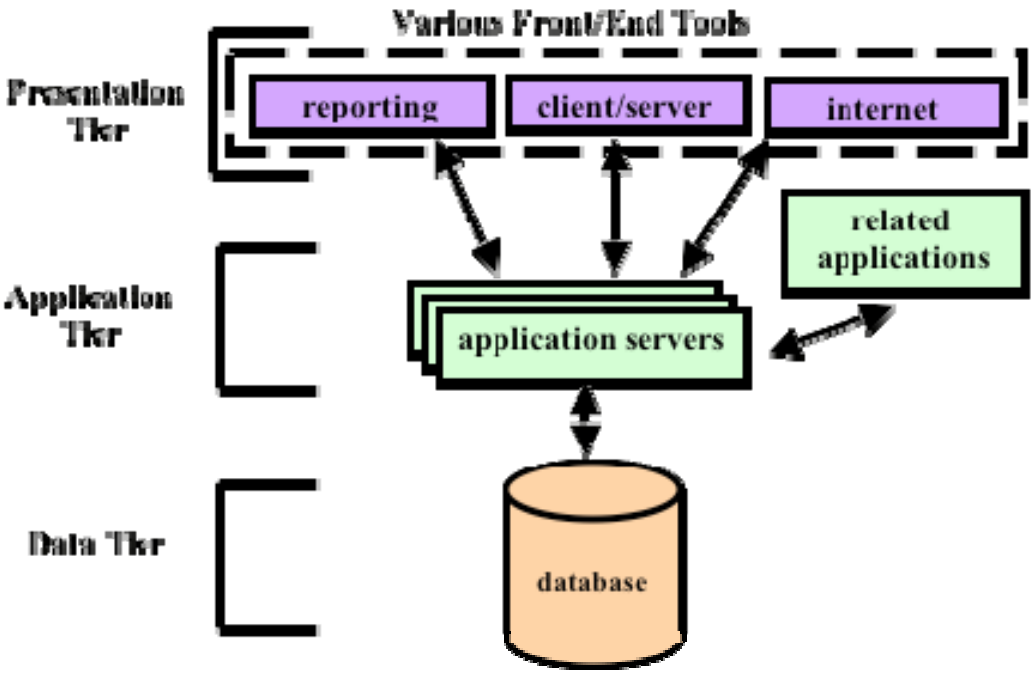

Figure 3. The Three-Tier/N-tier Model for Web-Accessible *Handbook*

4.2 Considerations for *Gen IV Materials Handbook* Web Site Development

Depending on the web developers and techniques they use, there are various approaches to construct a web-accessible database. For the *Handbook*, its development can be divided into the following phases:

Phase I - Detailed Product Analysis and Specification: This phase will focus on structural design of the web site, mainly on specifying the detailed structure of various tiers. It should yield three deliverables: 1) a product requirements document that details all the required functionalities and use case diagrams (This deliverable should be done mainly by the *Handbook* task, with inputs from the users, all the stakeholders, and some help from the web site developer); 2) an architecture and system design document which shows how data will flow from end to end (This is mainly the web site developer's responsibility); and 3) a User Interface (UI) specification document that describes the user interface specifications (This should be done through close collaboration between the web site developer and the *Handbook* task with input from the users and stakeholders).

Phase II - Simulation & Design: This phase will focus on designing all components of the model. High-level and low-level designs will be conducted on all participating servers. The interface definition will normally be discussed and documented during this design phase.

Phase III - Implementation & Testing: This phase will focus on detailed construction of the *Handbook***.** Every component program of the *Handbook* will be coded, individually and/or collectively tested, and then integrated into the model structure and certified.

Phase IV – Product Release: In this phase, the product will be launched with an initial compilation of data and released to the *Handbook* task and will allow users to login. Meanwhile, the web site developer will turn the web site over to a system support team that will monitor the servers continuously.

Phase V - Project/Product Evaluation: The *Handbook* users will send feedback to the web developer, and the quality of the product will be evaluated and improved.

Phase VI – Product Maintenance and Enhancement: New demands emerging from the Gen IV design process and rapid development of IT technologies will likely result in new requirements relative to functionalities and capacity enhancement. Additional data will be added. Updates will be made periodically to meet these new needs.

Depending on the developer eventually selected for the *Handbook*, the above phases may vary slightly but the basic procedures should be similar.

In order to develop the web-accessible *Handbook* economically and efficiently, it is an appropriate approach to contract web site development and/or maintenance to a private company or companies through bidding. The *Handbook* task will need to prepare, guide, and supervise the solicitation and bidding process. The preparation should include a clear description of the project, development strategies, solicitation for bidding, development of product requirements, award considerations and criteria, and a list of candidate contractors with their profiles.

Regarding the strategies for development contracting, there are three suitable options that should be reviewed and considered for hosting the database server. A decision will be made, early in the handbook development, on which hosting option will be used based upon the following considerations:

1) Self-hosting server
2) Co-located server
3) Virtual-hosting server

In the self-hosting server option, the Gen IV Program would own the machines and network hardware for the servers, and the servers would be located at a site selected by the Gen IV Program. The advantages of this option are several. First, the Gen IV Program would have full control of the servers. Second, if a national laboratory site such as ORNL, is selected for the server, the database is physically well secured. Third, if the servers are located at a national laboratory site, a strong in-house maintenance force is available. For example, the ORNL Computing and Computational Sciences Directorate conducts leading edge, state-of-the-art research and development in computer and computational sciences in support of DOE's missions and programs. One of the disadvantages of the self-hosting option is the higher cost of the machines and network hardware that must be purchased. Also, because the developer may be offsite, the developer will encounter certain inconveniences in operation monitoring, system updating, and server maintenance.

In the co-located server option, the Gen IV Program would own the machines and network hardware for the servers but the servers would be located at the developer's site. This option offers the Gen IV Program legal control of the servers and is convenient for the developer to monitor system operation, update the system, and provide maintenance to the servers. However, security of the information may become a concern because the real Gen IV materials data are exposed at the developer's site at all times. Further, the high expense of purchasing the machines and network hardware is still not avoided, plus it is difficult for the Gen IV Program to have physical control of the servers since the machines would be offsite.

In the virtual-hosting server option, the Gen IV Program would not own the machines and the network hardware for the servers. This option significantly reduces the upfront expense for purchase of the machines and networking hardware and it also offers the advantage that the maintenance and management of the servers is completely the responsibility of the developer or maintainer. However, the option has the disadvantages

of 1) limited access to the servers, 2) having to share the machines with other customers of the developer, and 3) potential questions of security of the database.

Unless initial cost is a much greater concern than other factors and database information sensitivity is not a serious issue, the virtual-hosting server option will not be seriously considered. (Whether or not this option will be more cost effective in the long term is also still an open question). If the machines and network hardware can be obtained in-house at a national laboratory at reasonable cost, the self-hosting server would be the most preferable option. This is especially true if physical security of the database and in-house maintenance is considered important. During the development period, all the software can be coded on the developer's machine at the developer's site. The *Handbook* task can provide the developer with a prototype database for coding the software, testing the server operations, and verifying the system functionalities. To ensure information security, the prototype database does not have to contain real Gen IV materials data. The prototype data can be artificially generated using a computer or extracted from open literature. Once the software is developed, tested, and certified, it can be loaded onto servers and the prototype database can be replaced by the real database for Gen IV reactor materials. To further ensure security in case of a fire, flood, or other unexpected disaster, and to guarantee a smooth operation in case of machine down time, a backup system can be put in place at a secondary site, such as Idaho National Laboratory (INL). Meanwhile, all of the original software and the prototype database will remain at the developer's site for future debugging and product enhancement. Since the servers at the developer's site will be operating only on the prototype database, security of the real Gen IV materials database will not be at risk.

If the self-hosting server option is to be adopted, compatibility of machines at the developer and national laboratory sites must be considered when selecting the developer. The considerations should also include compatibility of the operating systems on the end user's computers.

For the self-hosting server option, the prototype database should be prepared to meet several requirements. First, the prototype data must be representative of the real Gen IV materials data in characteristics such as value range, format (e.g., 2 E3 vs. 2,000, or 2 x 10^3), decimal places etc. Second, the prototype data must be distinctive and must not be easily mistaken for the real Gen IV materials data when they are being replaced by the real data. Finally, the servers and some other conventional means can be used to process the prototype data. Examining the two results can then test the server operation.

Another strategy that may be considered is that of "piecewise construction strategy". To ensure the quality of the web database, the development can be contracted in pieces over time. Technically, it is much easier for a developer to debug and fix problems in a small piece of the large database. Finding problems and trying to fix them when the entire system has already been built up may prove very difficult, if not impossible, or lead to a collapse of the system. Managerially, a result-based renewable contract can always serve as an impetus for a developer, and financially, the piecewise contracting strategy may

better fit into the uncertainty of the Gen IV Materials Program funding. Each contract can cover certain functionalities based on functional requirements priority.

Regarding the standards or criteria for developer selection, factors that should be considered include, but are not limited to, technology, background, stability, cost, quality and security control, and attitude toward cooperation as discussed below:

Technology – Advancement of the modern information technology (IT) industry is very dynamic with new technologies emerging at a pace faster than any industries in human history. Although it is almost impossible to predict what technologies will be available ten years down the road, it is very important that outmoded or fading technologies not be chosen for the *Handbook* database development because the Gen IV Program is expected to last at least more than one decade. This is a very long time for the IT industry. An inexpensive contract with outmoded or fading technologies will almost surely prove very costly in system updating and functionality enhancement in the long run.

Background - The background of the candidate companies should be carefully examined and considered. Many companies offering web-accessible database services actually have lost their capability to develop high-quality database software and mainly focus on selling data from databases they established in past years.

Stability – Due to the competitive nature of the IT industry and rapid changes in its technology, it is difficult to predict a company's future. However, stability of the developer is very important for the long-term well being of the *Handbook*. System updates and functionality enhancements would be severely obstructed should the developer withdraw from the business in future.

Cost – Although the cost may be driven down in a bidding process, it is very important to keep in mind that quality comes before cost. Designers of the Gen IV reactors will heavily rely on the quality of the database infrastructure developed. Because the *Handbook* may be shared with many other countries, the cost for the infrastructure may also be shared.

Quality and Security Control – Software coding is an intensive and complicated process. Coding error or hacking programmer can cause serious problems in future server operation. Every IT company has its own measures to ensure product quality and security. For example, some companies practice "Extreme Programming" in which programmers work in pairs on the same coding piece to prevent error and hacker programming. Due to the high quality and security required for the *Handbook*, the developer's measures for quality and security control would be closely examined and approved prior to award of the contact.

Attitude toward Cooperation – Significant interactions and communications among the *Handbook* task, users, stakeholders, and the developer are needed

during the development, system updating, maintenance, and enhancement. A cooperative developer will be crucial for the success of the task. In addition to considering cooperation demonstrated during the solicitation and bidding process, certain mechanisms of cooperation will be included in the contract to ensure a successful collaboration.

4.3 Development of *Gen IV Materials Handbook* Product Requirements

As opposed to a hard-copy materials handbook that only presents data in fixed formats, a web-accessible handbook has the advantage of being able not only to change its data presentation format as needed by re-arranging the data according to the user's instruction, but also to conduct various data processing and analysis tasks as needed. The details of how the data presentation format is changed and how the data are processed and analyzed depend mainly on the server functionalities developed and the search criteria defined. The functionalities and search criteria must reflect the needs and demands of the *Handbook* users. In Phase I of the project development, the *Handbook* task must make sure that the developer has gained a full understanding of the *Handbook* users' needs and demands. Developing a detailed product requirements document through close interactions and communications between the *Handbook* task (representing the users' needs) and the developer should do this. Although the development of a detailed product requirements document involves inputs from the developer, the *Handbook* task must provide significant information accurately defining the requirements for the product.

The most important components of a product requirements document include use-case diagrams and functional requirements tables. The use-case diagrams define the flow of data in the system. Compared to that of the functional requirements, the development of the use case diagrams relies relatively more on the developer. Figures 1 and 2 have given a preliminary presentation of the major data flows desired, and can be employed as a basis for the development of use case diagrams. The functional requirements tables contain the descriptions of functionalities desired from the servers. Like the use-case diagrams, only the major functions desired will be specified here to lay out the basis for future detailed requirements development.

Table 1 contains master functional requirements for the *Handbook*. Since it defines only the major functions desired for the web-accessible *Handbook* database, the table will be subjected to modifications when more inputs are collected from the *Handbook* users and stakeholders. In Table 1, the identification number (ID) for each requirement consists of an acronym of the table name and a series number with an increment of 10 so that new requirements can be inserted into relevant locations as needed in future. In addition to the ID, each requirement is given a priority index letter representing meanings described below:

- R Required Feature, for feature functionalities that must be included to be a usable product.
- H High Priority, for feature functionalities that are important.
- M Medium Priority, for feature functionalities that are desired.

L Low Priority, for feature functionalities that are possible extras.
F Future Enhancements, for feature functionalities that may be developed in future for enhanced performance.

Each requirement in Table 1 will be expanded into a detailed functional requirements table or tables as indicated in the comment column. At present, only the access authorization requirement is expanded in Table 2 to show an example. The rest of the master requirements will be expanded through collaboration between the *Handbook* task and the developer. To ensure all the needed functionalities are covered, it is necessary that the functional requirements tables be reviewed, modified, and approved by users and stakeholders of the *Handbook*.

Table 1. Master Functional Requirements Table (MFR)

ID	Priority	Description	Comment
MFR1000	R	Allow global access through the world wild web.	
MFR1010	R	Only authorized users can access a specific section or sections of the *Handbook* and all communication in the database system is protected.	Implemented by Product Security Functionality (PSF)
MFR1020	R	Allow user to select the data of interest for presentation. The categories of interest include material type, material product form, testing temperature, testing environment, etc.	
MFR1030	R	Allow data to be presented in a spreadsheet with the contents of columns and rows defined by user.	
MFR1040	R	Original data are stored in SI units. System allows user to conveniently display the data in other units of user's choice.	
MFR1050	R	A displayed data spreadsheet allows user to select columns to be plotted.	
MFR1060	R	Allow download - A displayed data spreadsheet can be downloaded to user's computer in popular file formats such as a Microsoft Excel. Displayed text, plots, and graphics can also be downloaded in their respective popular formats.	
MFR1070	H	User can click on a specific data point in a spreadsheet or a plot and be linked to the micrograph images of the data point if they are available.	
MFR1080	F	User can click on a specific data point in a spreadsheet or a plot and be linked to the original reference literature.	
MFR1090	R	Only authorized user can modify database. The modifications include input of new data, deletion of old data in an existing section, and creating new sections for data input.	
MFR1100	M	Displayed data can be conveniently exported to popular commercial software packages such as ANSYS and ABAQUS for analysis.	
MFR1110	R	Displayed data can be conveniently treated by included statistical analysis server.	
MFR1120	F	User can leave comments, including analysis results, on given data. Such user inputs are stored in a specified	

		section and should not affect the original *Handbook* data. However, the data commented on will be so indicated and other users can click on the indicator to bring up the comments to review.	
MFR1130	M	*Handbook* can recommend test matrices for generating new data considerations. Detail 1: User can select to extract test conditions that have already been tested from the existing data in the database (i.e., the test conditions of all the existing data can be displayed with the number of existing data points under each condition). Detail 2: In a specified section, user can input the data needs for a given material and service condition. Detail 3: User can select to display the conditions under which data are still needed for the desired service conditions (i.e., the *Handbook* can derive matrices from the information discussed in Details 1 and 2 to recommend testing conditions for new data that should be generated).	

Table 2. Functional Requirements Table for Product Security Functionality (PSF)

ID	Priority	Description	Note
PSF1000	R	Login and Authentication – All transactions, especially those of IDs, passwords, or authentication tokens over public networks such as the internet, must always be protected with encryption and/or other compensating control regardless of the type of user accessing the *Handbook*.	
PSF1010	R	Access Privilege – User can only access his/her authorized section of the *Handbook*.	
PSF1020	H	User Login Records – All logins should be recorded with user IDs, time, and location of the user if possible.	
PSF1030	M	Database management is alarmed for unauthorized login attempts that have repeated more than three times. The time, possible location, attempted ID and password is recorded.	
PSF1040	R	Personal Identifying Information - transactions must always be protected with encryption or other compensating control. User's information (e.g., addresses, phone numbers, etc.) never goes over a public wire (internet) in the clear.	
PSF1050	R	User Communication - transactions must always be protected with encryption or other compensating control.	
PSF1060	R	Search and Information Retrieval - transactions should always be protected with encryption or other compensating control. Web Browsers and Servers should be set for mandatory security using the highest strength encryption available by law.	

5. Applicability of the Gen IV Materials Handbook

5.1 *Gen IV Materials Handbook* Stakeholders

The data and information included in the *Handbook* will be responsive to the needs expressed by all of the *Handbook* stakeholders. At the upper level, the stakeholders are the Gen IV Reactor Systems and potentially the NHI, and AFCI programs. At a lower level, using Gen IV Reactor systems as an example, stakeholders include Gen IV SIMs and researchers, DOE-NE, NRC, and potential reactor system designers and suppliers. Representatives of codes and standards bodies are also stakeholders in the *Handbook* in that data incorporated into the *Handbook* may eventually come to their attention for codes and standards approval. Stakeholders should also eventually include international partners through International Nuclear Energy Research Initiative (I-NERI) projects and Generation IV International Forum (GIF) implementing agreements.

The data and information provided through the *Handbook* is intended to be used by all stakeholders involved is the design, analysis, etc. of Gen IV Reactor Systems, the NHI, and AFCI. (Note that the AFCI has prepared and maintains a materials handbook but will give strong consideration to merging it with the *Handbook*.) Data provided will be taken from the latest and best information available and will permit vendors and clients to compare designs and evaluate performance on a consistent basis even though the materials under consideration may not currently be codes and standards accepted.

5.2 Quality Considerations for *Gen IV Materials Handbook* Data

The data provided in the *Handbook* will be identified and classified as follows.

Class 1 – These materials data meet all DOE Gen IV Reactor Programs and NRC QA requirements (i.e., these are data generated in documented R&D programs that meet all of the requirements of 10CFR50 Appendix B and DOE/NRC agreed versions of NQA-1). It is expected that the new data generated in Gen IV materials programs will be of this category. Data with this pedigree, it is assumed, would be entirely acceptable to DOE, NRC, and reactor vendors for use in final design and design analyses, especially if they are submitted to and approved by appropriate codes and standards bodies.

Class 2 – Materials data and data correlations provided in various sections of well-recognized U.S. codes and standards (e.g., ASME and ASTM) will be designated as Class 2. In many cases the raw data (i.e., individual data points) will not be available from these sources. Thus, the results of peer-approved analyses and resulting data correlations contained in these codes and standards may be the major Class 2 input to the *Handbook*. Further, although materials and materials data approved by codes and standards bodies are generally a necessary condition for acceptance of designs by State and Federal regulatory bodies, there may in some cases be additional requirements.

Class 3 – Materials data provided in well-recognized international codes and standards will be categorized at present as Class 3. This may be revisited as the result of any international agreements reached relative to cooperation on the *Handbook*. For example, such agreements might result in Classes 2 and 3 being combined into a single class.

Class 4 – Materials data obtained from materials handbooks such as the *Nuclear Systems Materials Handbook* and the *AFCI Materials Handbook* will be identified as Class 4. The data contained in these two examples have had careful and extensive analysis and peer review (equivalent to Class 2) but the data were generated under quality conditions ranging from "unknown" to equivalent to Class 1. In the latter case, the data from such handbooks would be listed as Class 1.

Class 5 – Materials data obtained from sources such as manufacturers brochures and the open literature will be categorized as Class 5. Such data will, of course, be reviewed and approved before it is incorporated into the *Handbook*.

Although the classifications described above are not an absolute measure of the quality of data, they do provide a "standard" basis for guidance on data acceptability and assurance. Further, questions relative to data uncertainties and ranges will be addressed in the *Handbook* by providing individual data points (whenever possible), including a characterization of each data point in terms of material and test parameters, source, and incorporating software packages for statistical analysis.

5.3 Identification of *Gen IV Materials Handbook* Materials and Data Requirements

In order to maintain the responsiveness of the *Handbook* to stakeholders, the *Handbook* must be positioned to respond quickly and efficiently to changing requirements relative to materials and materials data of interest. The entity charged with the ongoing identification of materials and materials data needed in the *Handbook* is the Gen IV Materials Handbook Advisory Group (Advisory Group) to be discussed under Organizational Structure. Incorporation of the materials and materials data identified by the Advisory Group into the *Handbook* will be implemented through operation of the portions of the Organizational Structure responsible for *Handbook* preparation, publication, and distribution.

6. Organizational Structure of the Gen IV Materials Handbook

An overview of the proposed overall organizational structure of the *Handbook* is presented in Figures 4, 5, and 6. The "top level" organizational structure is shown in Figure 4 and discussion is provided below relative to each of the boxes/positions. Figures 5 and 6 provide details of the organizational structures of *Handbook* Volume I (Metals) and Volume II (Non-Metals), respectively. Description is also provided as to the duties and responsibilities of the positions represented by the various boxes.

The *Handbook* will be sponsored by and responsive to DOE-NE management (see Figure 4) and will be under the purview of the Gen IV Materials National Technical Director (NTD). The overall responsibility for the *Handbook* will fall to a "Manager of Operations". This position will manage and control all *Handbook* operations and have the final sign-off on all data and information incorporated into the *Handbook*. The "Manager of Operations" will receive and be responsive to the continuing advice of an Advisory Group as to content and operation of the *Handbook*. The "Manager of Operations" will also receive and be responsive to continuing input from a "Manager of Quality Assurance".

The Advisory Group will be the primary means of representing the interests of the large number of stakeholders with respect to the *Handbook*. At the program level, these stakeholders include Gen IV Reactor Program, the NHI, and the AFCI. Specific to the Gen IV Reactor Program, for example, stakeholders include DOE, the NRC, appropriate codes and standards representatives, Gen IV Programs SIMs, Gen IV Materials Program management, and potential Gen IV reactor systems designers and vendors. The needs and requirements of all of the stakeholders relative to information and materials needed in the *Handbook* will be handled through the participation of representatives of the stakeholders in the Advisory Group.

"Oversight Managers" for Volume I (Metals), Volume II (Non-Metals), and for *Handbook* on-line inputs and control will report directly to the *Handbook* "Manager of Operations" (see Figure 4). The "Oversight Manager" for Volume I (Metals) of the *Handbook* has oversight responsibility for the preparation, review, and submission of all data and information on metals to be incorporated into the *Handbook*. Selection of the materials and materials data and information to be included in Volume I will flow down to the "Oversight Manager" from the "Manager of Operations" of the *Handbook*. The "Oversight Manager" is also responsible for organizing peer reviews of the user inputs (i.e., comments and analysis results on data in the volume under his/her charge) and accepts, rejects, or advises revising the comments based on the peer review.

The *Handbook* Volume I (Metals) "Oversight Manager" will be assisted by six "Assistant Managers" corresponding to the metallic material categories identified earlier in this document. As shown in Figure 5, these "Assistant Managers" will be responsible, respectively, for the materials categories "ferritic alloy steels" (e.g., SA 533 Grade B Class 1), "ferritic-martensitic steels" (e.g., T91), "austenitic stainless steels" (e.g., 316 H), "Ni- and Co-base alloys" (e.g., Hastelloy X), "refractory and other alloys" (e.g., W), and "welding filler metals". The "Assistant Managers" will be responsible for seeing that all of the data and information required for each of the materials in their categories are collected, analyzed, arranged in the proper format for the *Handbook*, reviewed by an appropriate group of individuals, and forwarded to the "Oversight Manager" for his approval. They will also be responsible for preparing the *Handbook* sections relative to general information (e.g., alloy chemistry and specifications) for each of the materials under their charge. "Task Leaders" competent in the areas of mechanical properties, physical and thermal properties, corrosion and environmental effects, and radiation

effects will aid each “Assistant Manager” by collecting relevant data and information and preparing the *Handbook* sections relative to their areas of expertise.

A “Manager of On-line Inputs and Control” will also report to the *Handbook* “Manager of Operations”. This position will be responsible for all of the mechanics of input, maintenance, and control of the web-based *Handbook.* The exact scope and scale of these responsibilities will be established as part as the ongoing assessment of web site development for the *Handbook*.

Figure 6 illustrates the organizational structure of Volume II (Non-Metals) of the *Handbook*. Similar to the Volume I organizational structure discussed above, the Volume II “Oversight Manager” is assisted by “Assistant Managers”. The two “Assistant Managers” are responsible for “Graphites and Carbon Composite Materials” and “Ceramic and Ceramic Composite Materials”, respectively. These “Assistant Managers” oversee the activities of “Task Leaders” representing the areas of mechanical properties, physical and thermal properties, corrosion and environmental effects, and radiation effects, respectively. The duties and responsibilities of the Volume II positions mirror those discussed for Volume I.

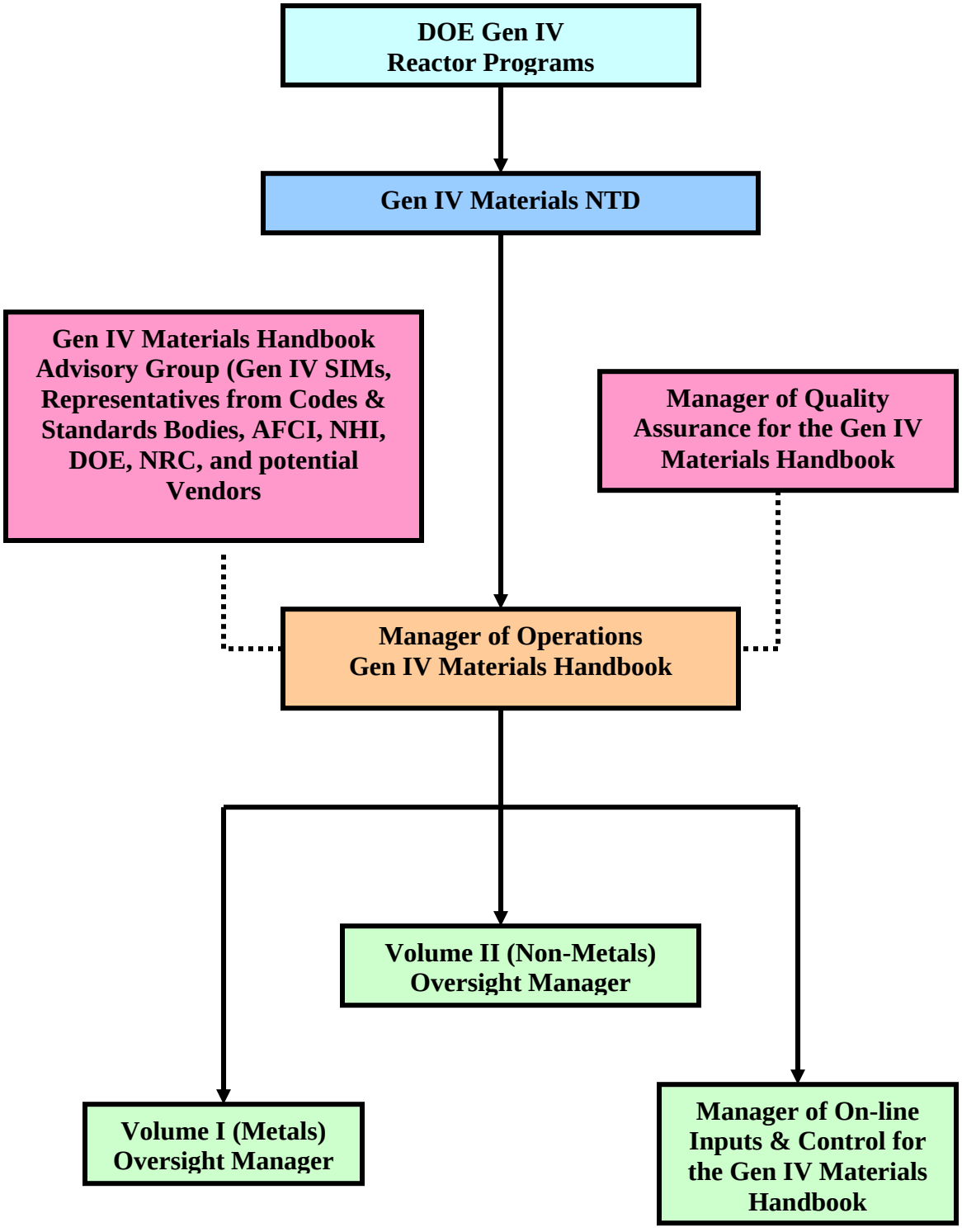

Figure 4. Top Level Organizational Structure for the Gen IV Materials Handbook

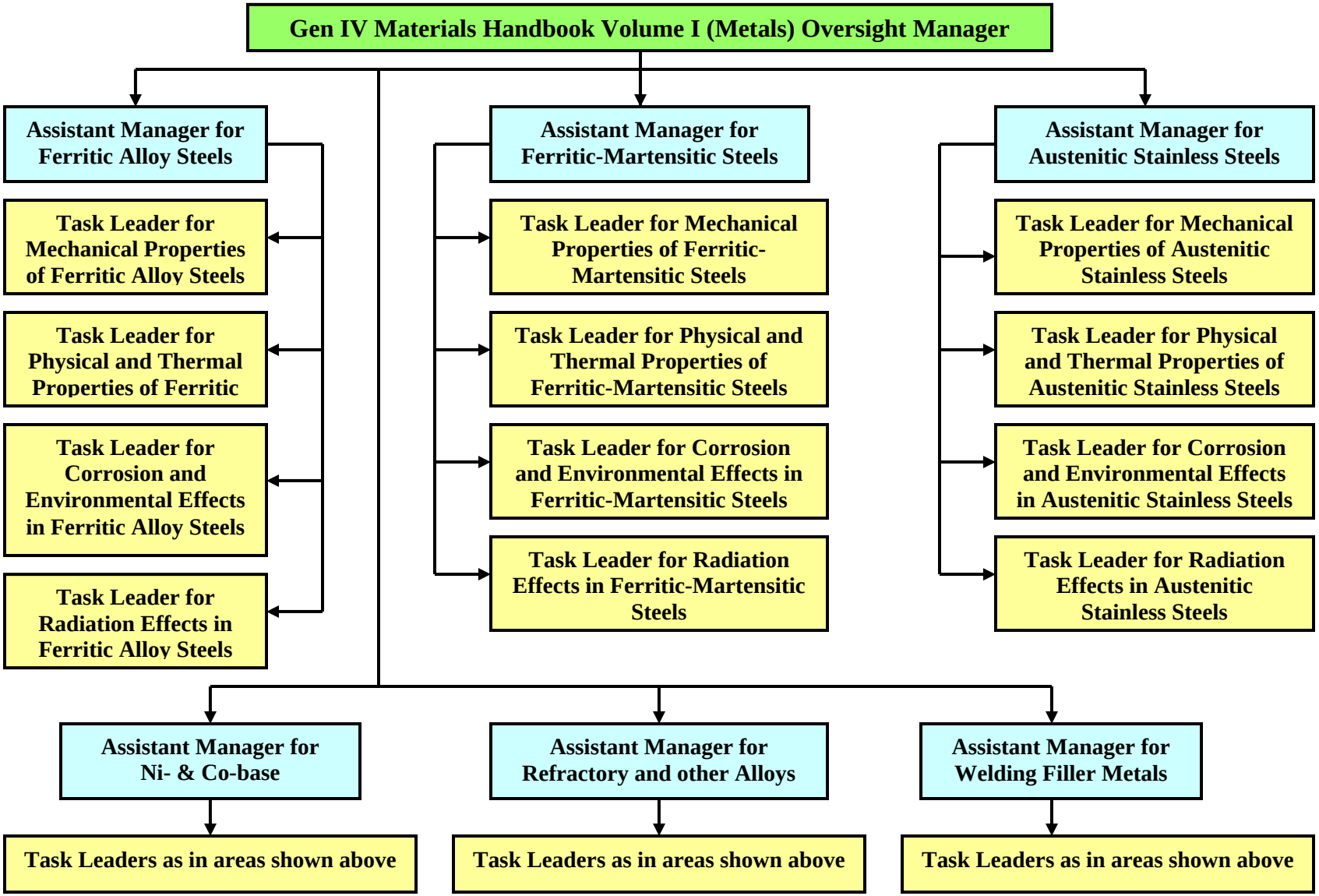

Figure 5. Working Level Organizational Structure for Volume I of the Gen IV Materials Handbook

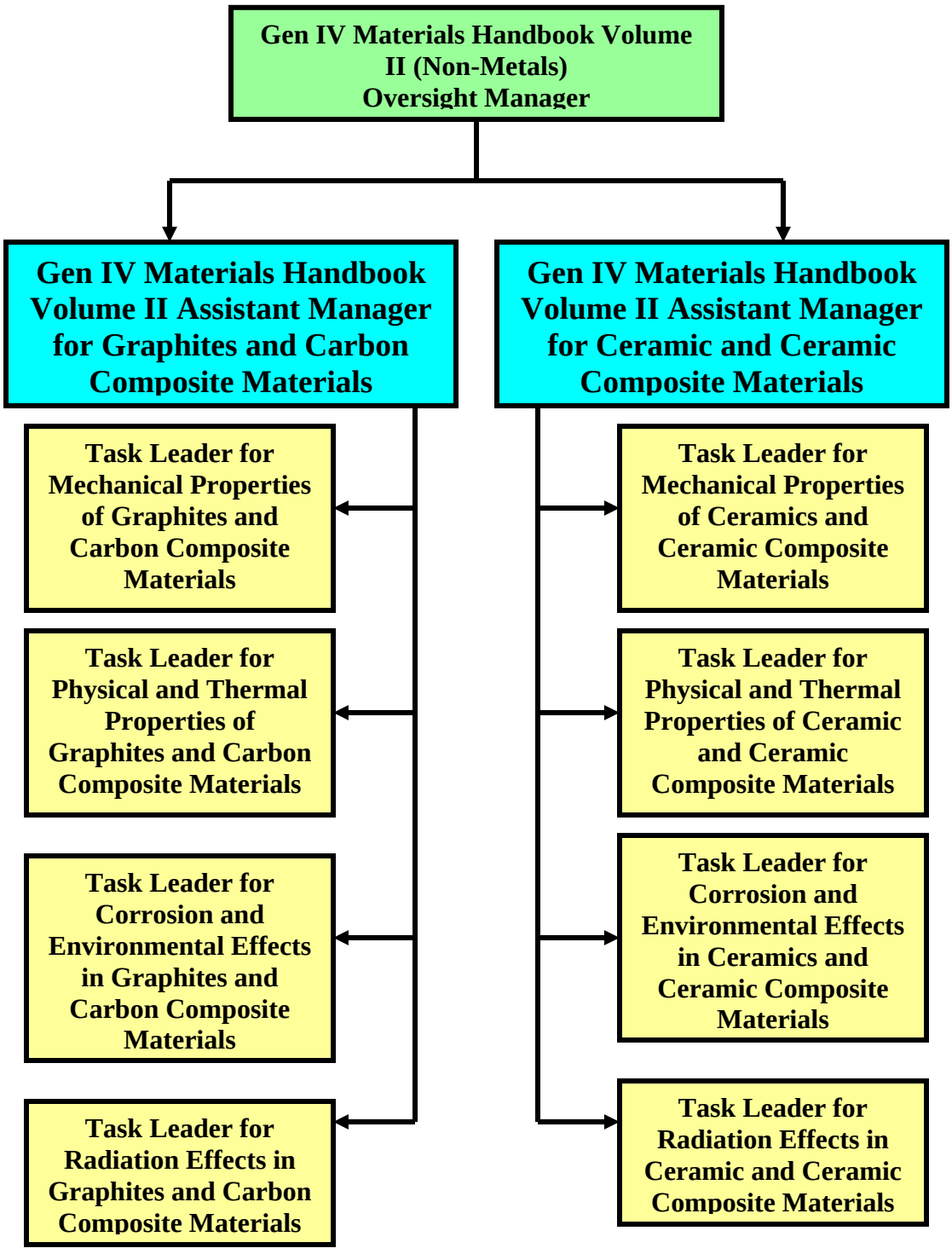

Figure 6. Working Level Organizational Structure for Volume II of the Gen IV Materials Handbook

7. Preparation, Publication, and Distribution of the Gen IV Materials Handbook

7.1 Preparation

Materials experts from national laboratories, universities, and other organizations involved in Gen IV Reactors, NHI, and AFCI will prepare the materials data and information contained in the *Handbook*. The materials sections and materials data and information to be prepared for the *Handbook* will be prescribed by the Gen IV Materials Handbook "Manager of Operations" based on the advice of the *Advisory Group*. The charge to prepare these sections for the *Handbook* will feed down to the "Oversight Managers" of *Handbook* Volume I and Volume II. The "Oversight Managers" have the overall responsibility for the preparation and review of all *Handbook* inputs related to their areas and submission of these to the "Manager of Operations" for approval. The detailed preparation of *Handbook* inputs for specific areas (e.g., ferritic alloy steels) will be delegated to an "Assistant Manager", in this case the "Assistant Manager for Ferritic Alloy Steels". The "Assistant Managers" for each material category in each *Handbook* volume (see Figures 5 and 6) will further delegate preparation of inputs for the *Handbook* to "Task Leaders" in the areas of mechanical properties, physical and thermal properties, corrosion and environmental effects, and radiation effects. These "Task Leaders" may form teams of materials specialists to participate in the preparation of *Handbook* inputs.

The procedure described above for materials inputs prescribed by the "Manager of Operations" can be summarized as follows.

- "Task Leaders" and their teams prepare the inputs relative to their areas of expertise.
- The "Assistant Managers" for each material category collate the inputs received from the "Task Leader" teams and forward them to the appropriate "Oversight Manager".
- The "Oversight Manager" ensures that the *Handbook* inputs received undergo thorough peer reviews and, when all review comments are reconciled, forwards the *Handbook* inputs to the "Manager of Operations" for final approval.

7.2 Publication

After the *Handbook* "Manager of Operations" approves a package of inputs, he/she directs **t**he *Handbook* "Manager of On-line Inputs and Control" to provide for entering the submittals into the web-based *Handbook*. All of the data and information becomes immediately available to all stakeholders subject to controls discussed earlier.

7.3 Distribution

The distribution of the *Handbook* will be restricted to stakeholders and controlled by passwords issued to individuals with the approval of the *Handbook* "Manager of

Operations". Members of the *Advisory Group* or any organization participating in Gen IV, NHI, or AFCI programs may make requests for passwords to the "Manager of Operations".

8. Quality Assurance for the Gen IV Materials Handbook

8.1 General

Quality Assurance will be conducted in strict compliance with References 4 and 5, as well as additional Gen IV Program QA Requirements as they are developed.

8.2 Website Software Quality

The website software design requirements will be identified and documented. Software design requirements will identify the operating system, function, interfaces, performance requirements, and any constraints of the system selected. The design will be documented, reviewed, and approved. The software will be verified by testing using the prototype data provided by the Gen IV Program. After the baseline is established, configuration management, which includes version identification, change control, and status control, will be applied to the website software for the *Handbook*.

8.3 Data Quality

All data presented in the *Handbook* will be identified with its quality level. A plan will be developed for verification of the data inputs. Verification of the data inputs and their quality level will be accomplished prior to inclusion into the *Handbook* and records of that verification maintained.

8.4 Records

Records will be maintained for:

- Website software design and verification
- Configuration control of the website application software.
- Materials data and validation

Records will be protected in accordance with the NGNP Materials Quality Assurance Plan.

9. References

1. William R. Corwin, Updated Generation IV Reactors Integrated Materials Technology Program Plan, Revision 1, ORNL/TM-2003/244/R1 (Draft), August 31, 2004.

2. William Corwin, et. al., Materials Requirements for Nuclear Hydrogen Generation Systems, ORNL/TM-2004/DRAFT, September 21, 2004.

3. Stuart Maloy, “Letter Report on Gen IV Reactor Materials”, LANL, LA-UR-03-4648, July 28, 2003.

4. QAP-ORNL-NGNP-01, Quality Assurance Plan for the NGNP Materials Program at ORNL.

5. PLN-1792, Quality Program Plan for NGNP Materials R&D Program.